

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040820\
 Data File : BF119872.D
 Acq On : 9 Apr 2020 16:30
 Operator : MA/SJ
 Sample : L2135-02
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-2J-(0-2)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.975	486	491	497	rVB	122974	153640	3.02%	0.436%
2	5.381	555	560	563	rBV	3740791	3484763	68.61%	9.879%
3	6.404	728	734	737	rBV	3785512	4243684	83.55%	12.031%
4	6.592	764	766	772	rBV	100501	95845	1.89%	0.272%
5	6.763	792	795	799	rBV	1191557	1065510	20.98%	3.021%
6	6.922	818	822	826	rBV	3591991	3502190	68.95%	9.929%
7	7.334	886	892	895	rBV	3098355	2935829	57.80%	8.323%
8	8.051	1009	1014	1017	rBV	1670107	1324436	26.08%	3.755%
9	9.133	1192	1198	1201	rBV	6049763	5079197	100.00%	14.399%
10	9.522	1261	1264	1268	rBV	704441	590156	11.62%	1.673%
11	9.810	1307	1313	1316	rBV	1657992	1402811	27.62%	3.977%
12	10.598	1442	1447	1450	rBV	2597275	2279513	44.88%	6.462%
13	11.292	1561	1565	1569	rBV	1593113	1331973	26.22%	3.776%
14	11.827	1653	1656	1667	rBV	339900	334545	6.59%	0.948%
15	12.539	1768	1777	1787	rBV2	467365	702556	13.83%	1.992%
16	12.616	1787	1790	1796	rVV	192133	212481	4.18%	0.602%
17	12.886	1831	1836	1839	rBV	3915190	3353224	66.02%	9.506%
18	13.363	1910	1917	1923	rBV2	130643	175894	3.46%	0.499%
19	13.792	1987	1990	2001	rVB	146270	217854	4.29%	0.618%
20	13.933	2010	2014	2017	rBV	1055520	894259	17.61%	2.535%
21	14.110	2040	2044	2047	rBV	111909	106628	2.10%	0.302%
22	14.410	2091	2095	2099	rBV	159293	179974	3.54%	0.510%
23	14.715	2143	2147	2150	rVB	186401	177409	3.49%	0.503%
24	15.045	2199	2203	2206	rVB	180569	209486	4.12%	0.594%
25	15.368	2254	2258	2262	rBV	685356	797236	15.70%	2.260%
26	15.410	2262	2265	2274	rVB	137361	189582	3.73%	0.537%
27	15.833	2332	2337	2344	rVB	94688	145199	2.86%	0.412%
28	16.321	2415	2420	2425	rVB2	54024	87676	1.73%	0.249%

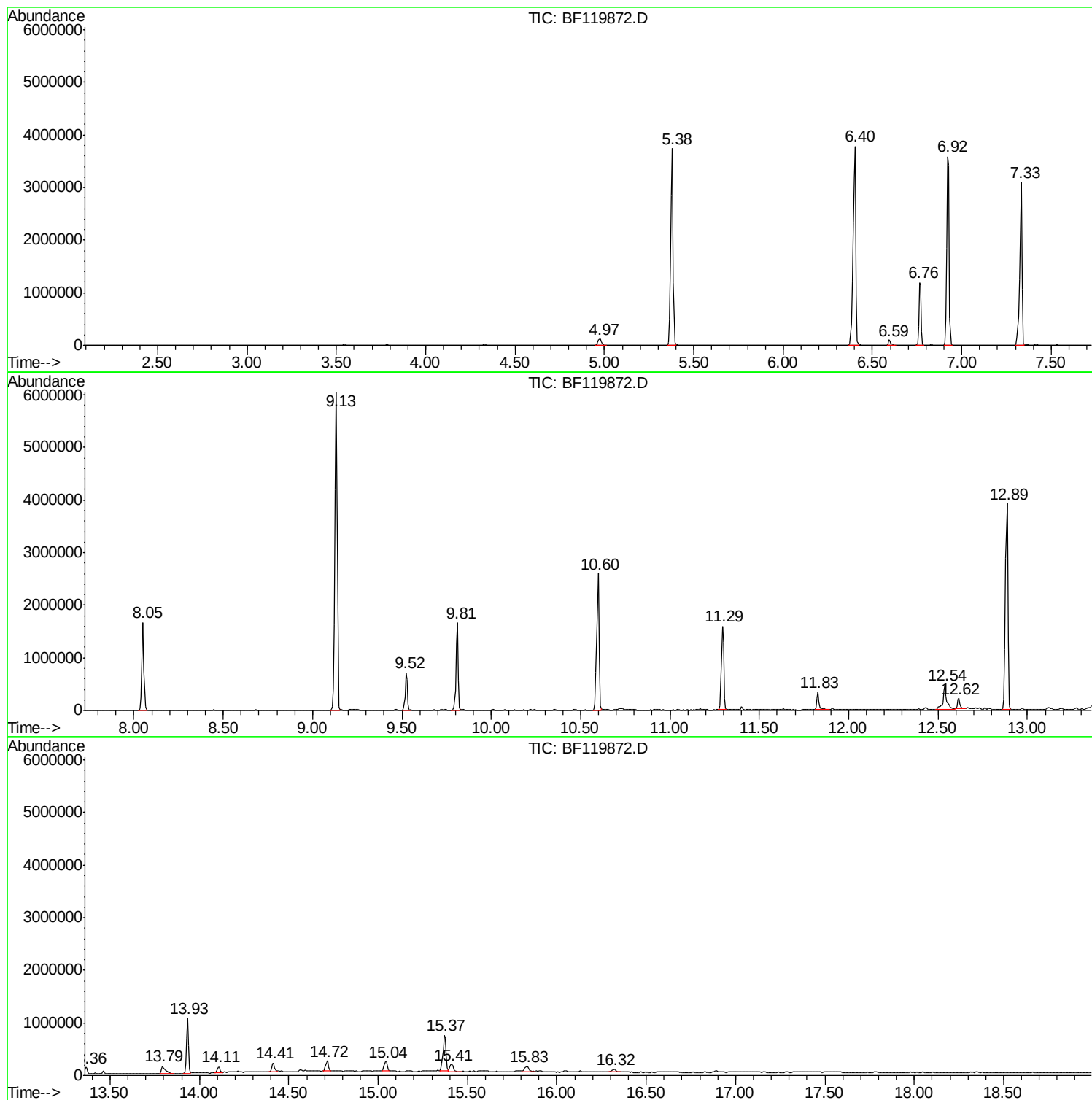
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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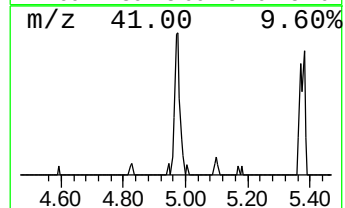
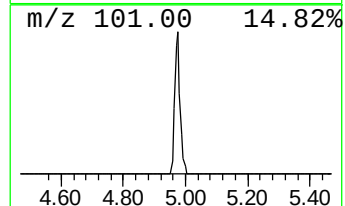
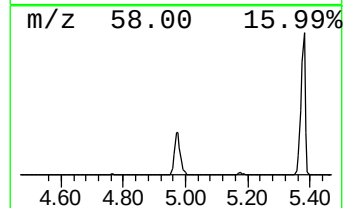
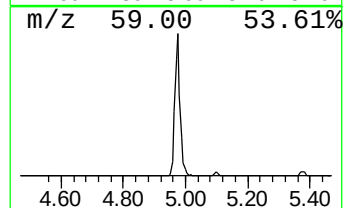
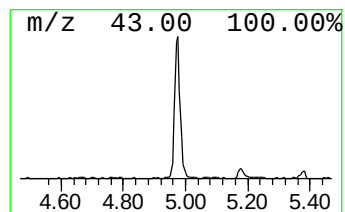
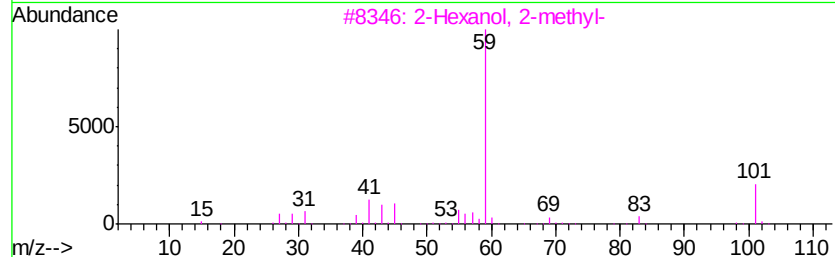
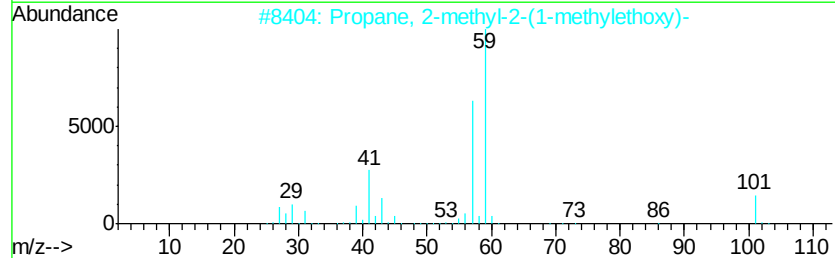
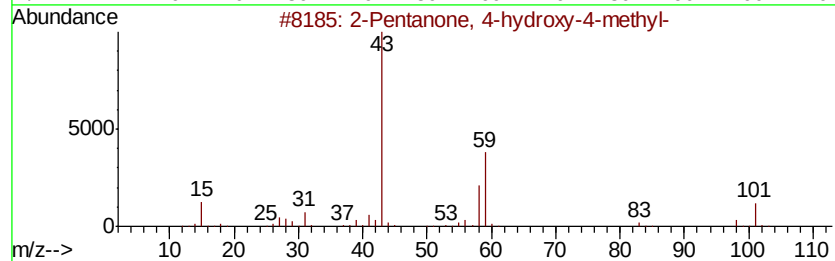
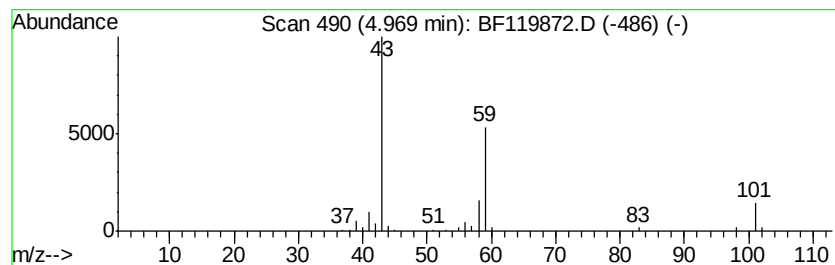
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	2.88 ng	153640	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol	102	C6H14O	000623-37-0	33
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28



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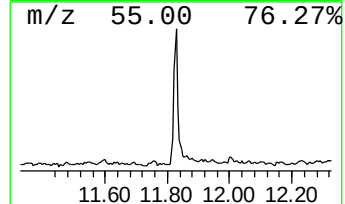
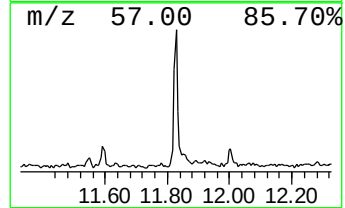
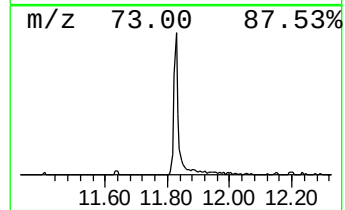
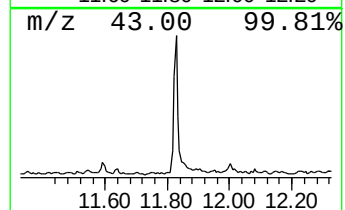
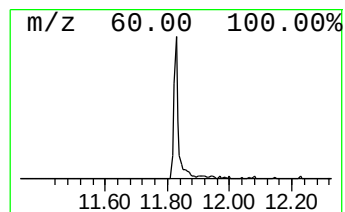
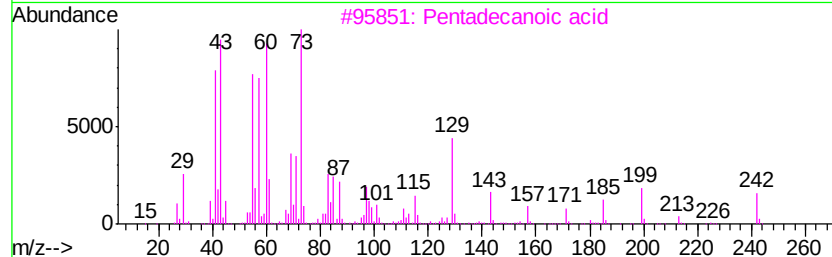
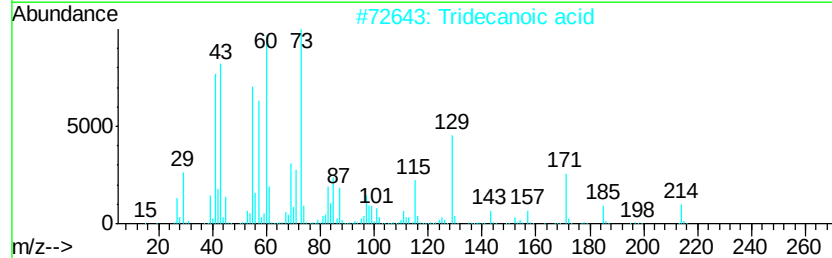
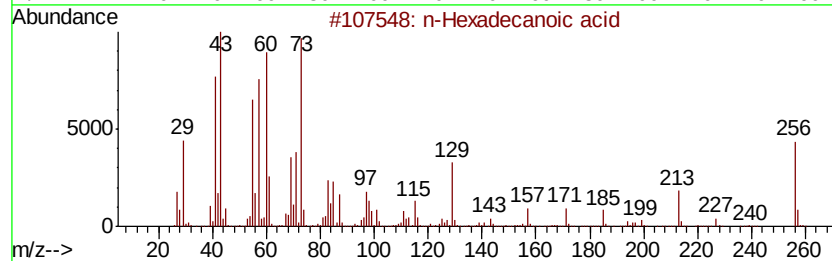
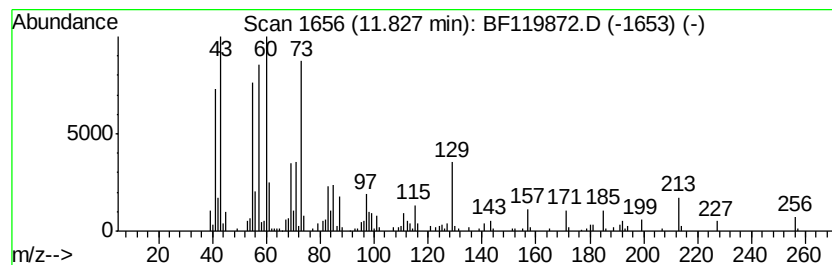
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.83	5.02 ng	334545	Phenanthrene-d10	11.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53



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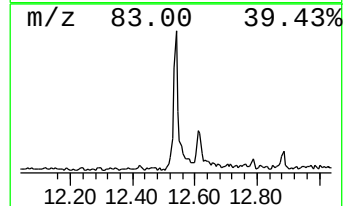
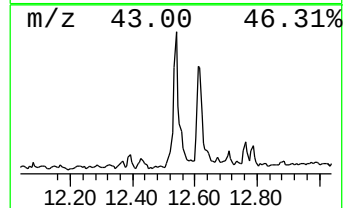
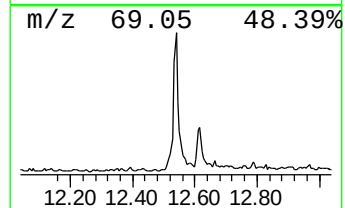
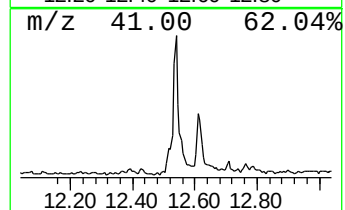
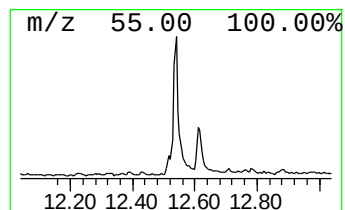
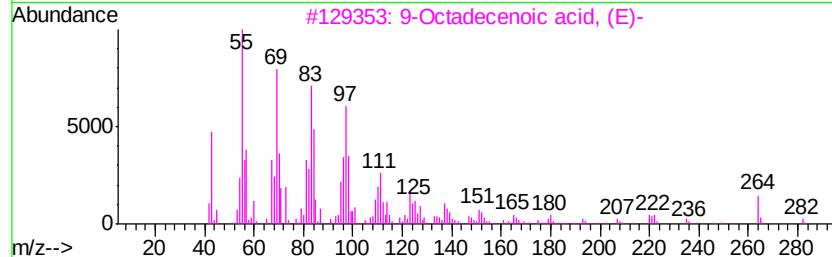
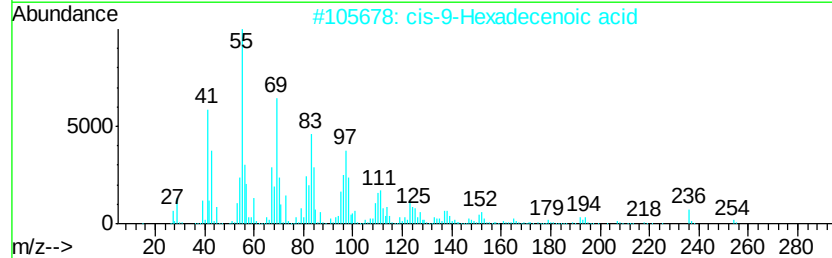
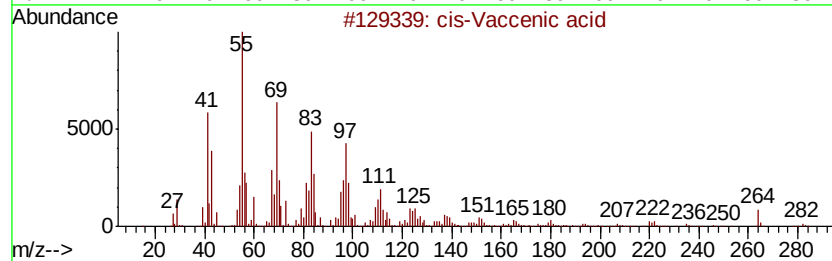
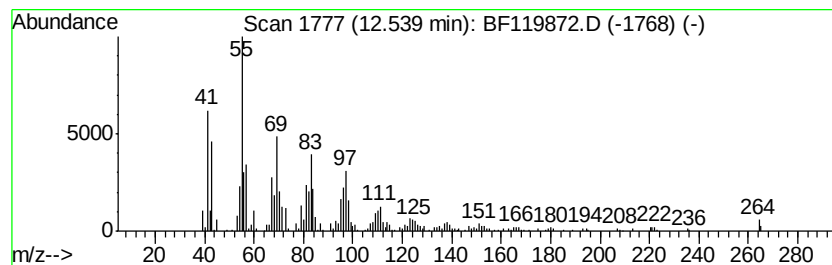
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Peak Number 4 cis-Vaccenic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.54	10.55 ng	702556	Phenanthrene-d10	11.29		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
2		cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	90
3		9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	90
4		Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	90
5		9-octadecanoic acid, 2,2,3,3,4,4...	464	C22H35F7O2	1000376-61-4	90



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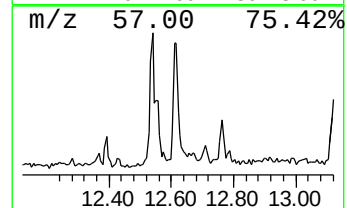
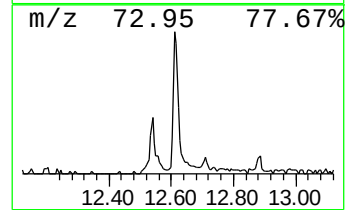
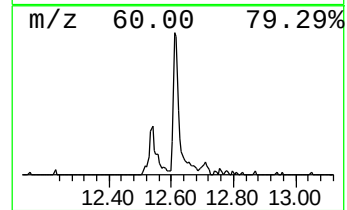
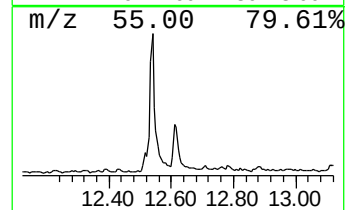
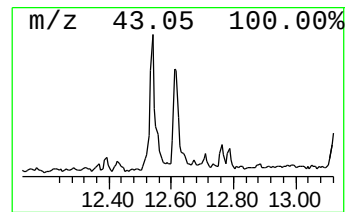
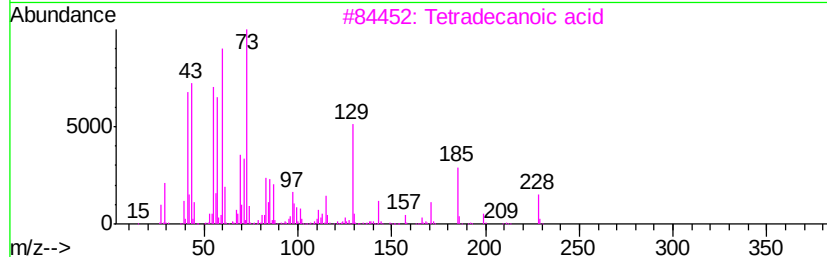
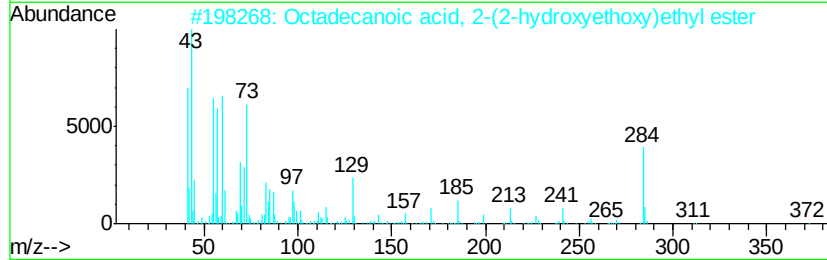
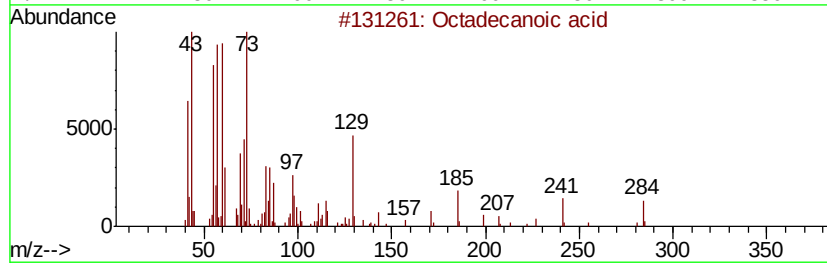
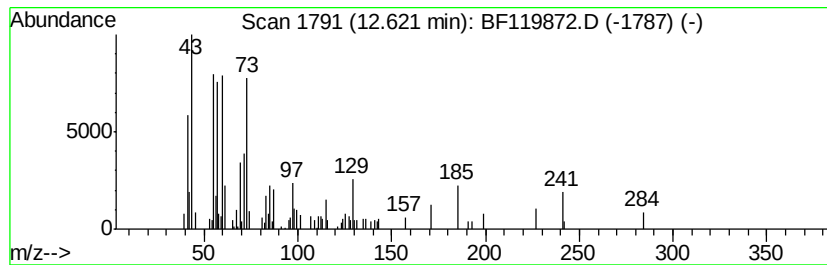
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	4.75 ng	212481	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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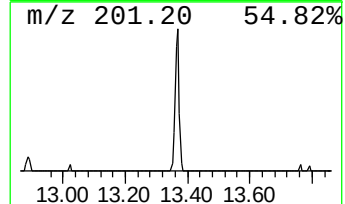
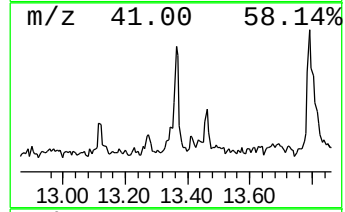
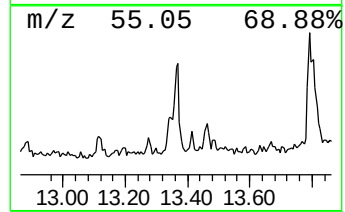
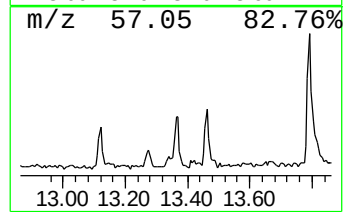
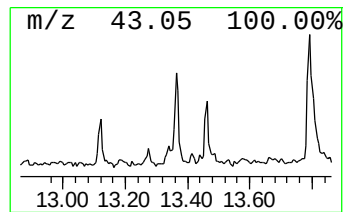
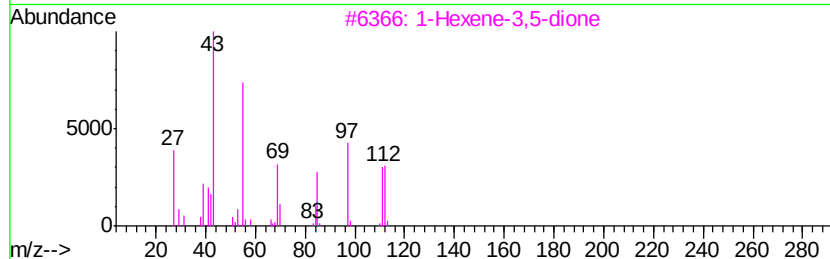
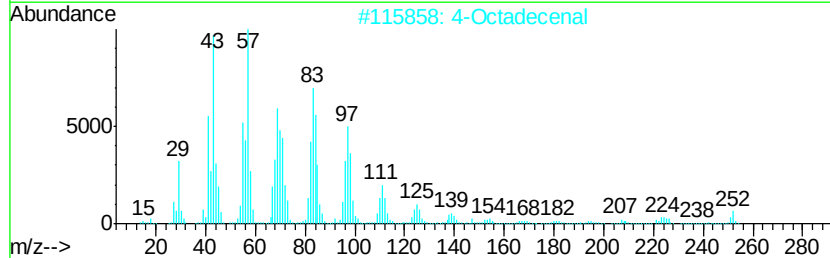
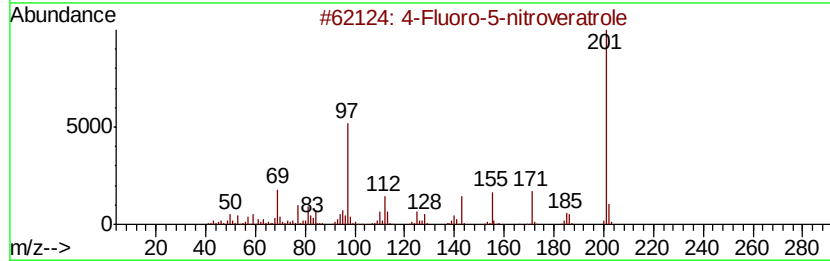
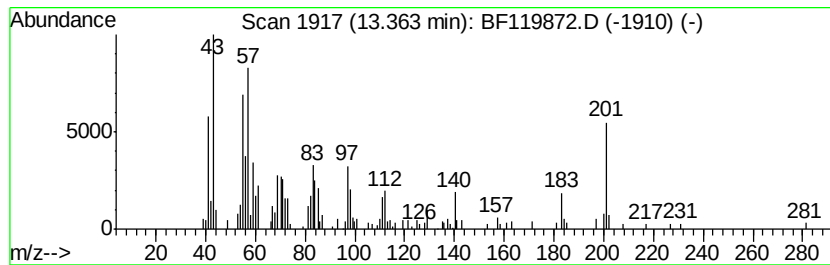
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Peak Number 6 unknown13.36 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.36	3.93 ng	175894	Chrysene-d12		13.93
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Fluoro-5-nitroveratrole	201	C8H8FN04	1000257-02-6	25
2	4-Octadecenal	266	C18H34O	056554-98-4	25
3	1-Hexene-3,5-dione	112	C6H8O2	052204-69-0	22
4	Cyclodecane	140	C10H20	000293-96-9	18
5	1-Dodecene	168	C12H24	000112-41-4	18



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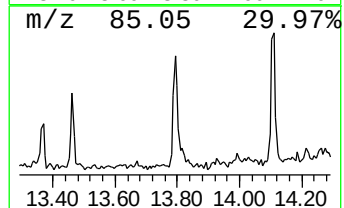
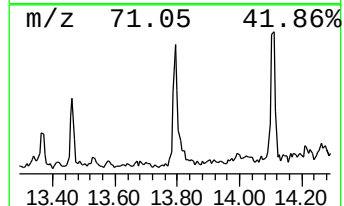
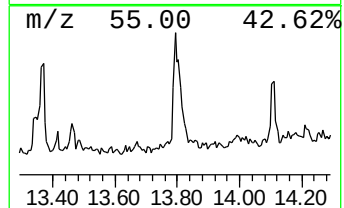
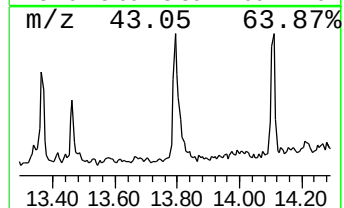
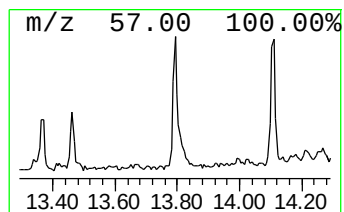
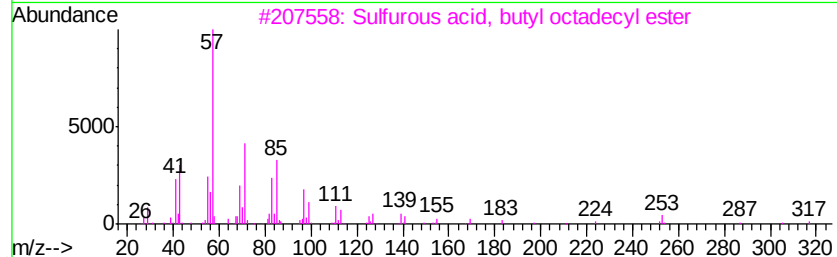
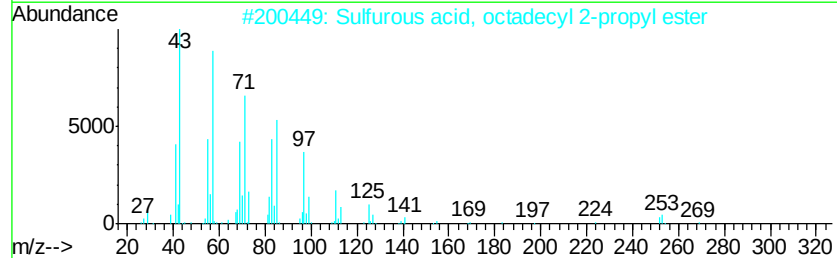
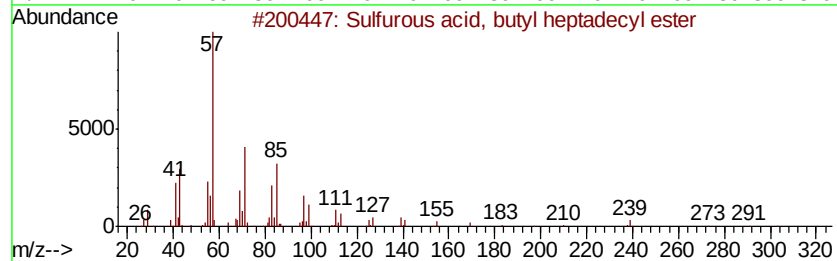
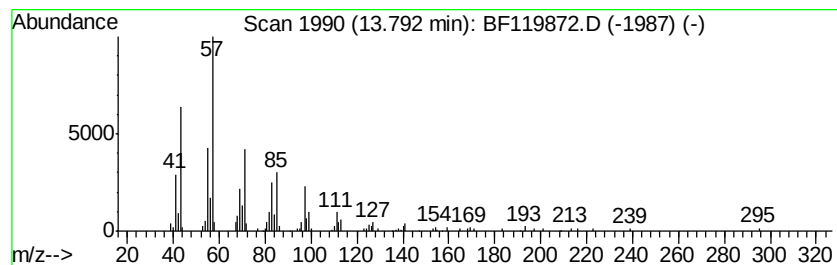
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Sulfurous acid, butyl hepta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	4.87 ng	217854	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	87
2		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
3		Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	86
4		Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	86
5		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040820\
Data File : BF119872.D
Acq On : 9 Apr 2020 16:30
Operator : MA/SJ
Sample : L2135-02
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2J-(0-2)

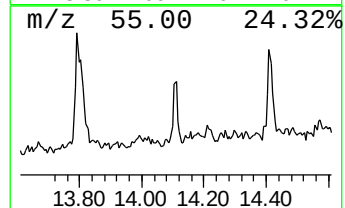
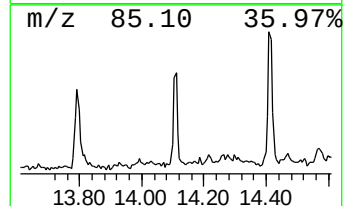
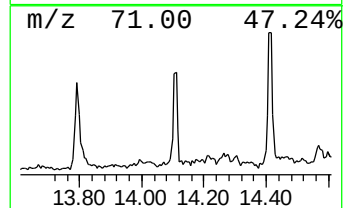
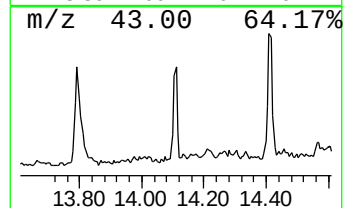
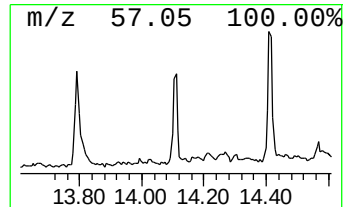
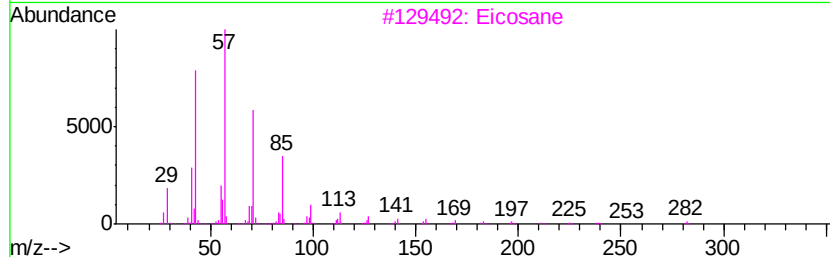
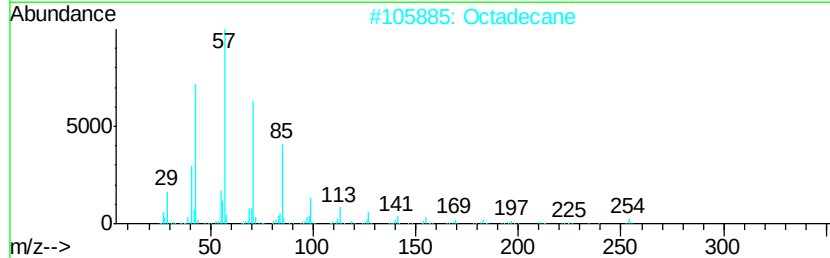
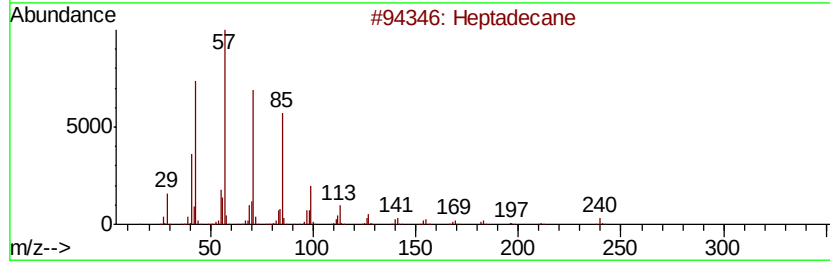
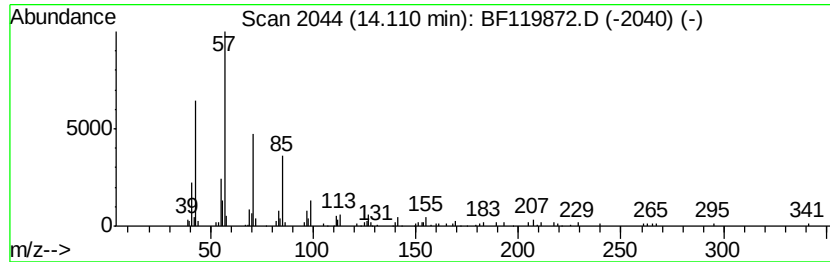
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.11	2.38 ng	106628	Chrysene-d12	13.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	94
2	Octadecane		254	C18H38	000593-45-3	83
3	Eicosane		282	C20H42	000112-95-8	83
4	Tetracosane		338	C24H50	000646-31-1	83
5	Heneicosane		296	C21H44	000629-94-7	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040820\
Data File : BF119872.D
Acq On : 9 Apr 2020 16:30
Operator : MA/SJ
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Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-2J-(0-2)

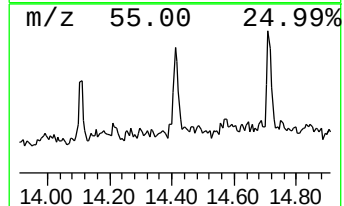
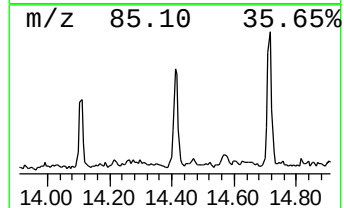
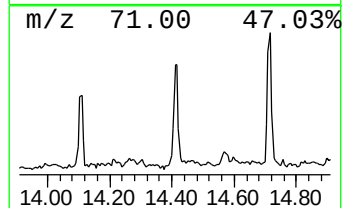
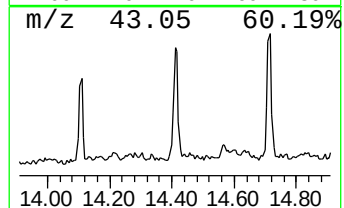
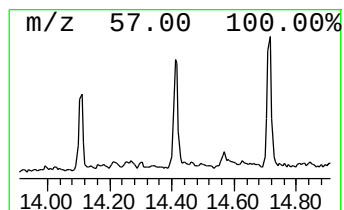
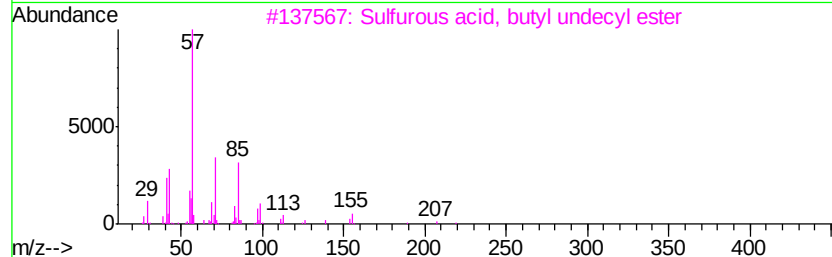
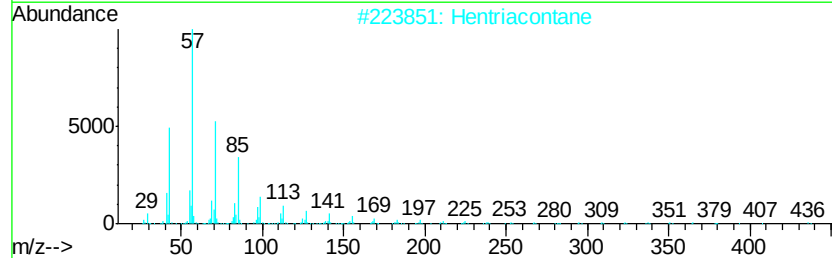
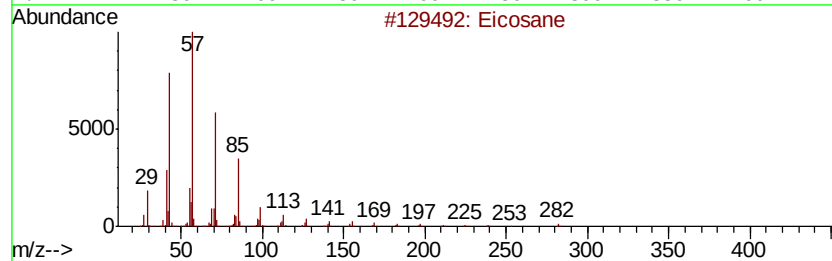
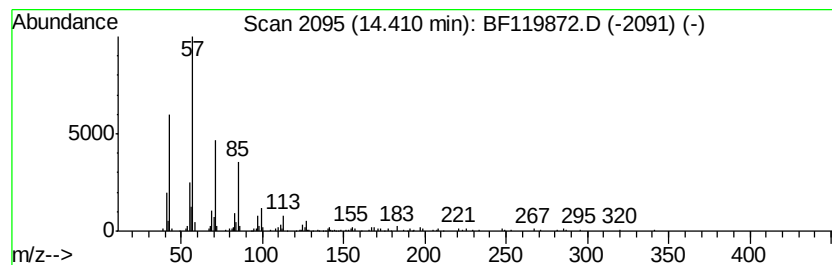
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	4.03 ng	179974	Chrysene-d12	13.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	90
2	Hentriacontane		437	C31H64	000630-04-6	86
3	Sulfurous acid, butyl undecyl ester		292	C15H32O3S	1000309-17-8	86
4	Heneicosane		296	C21H44	000629-94-7	83
5	Tetratetracontane		619	C44H90	007098-22-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040820\
Data File : BF119872.D
Acq On : 9 Apr 2020 16:30
Operator : MA/SJ
Sample : L2135-02
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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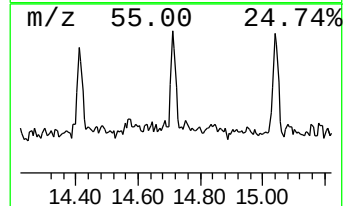
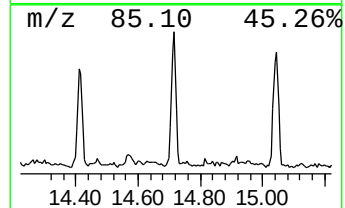
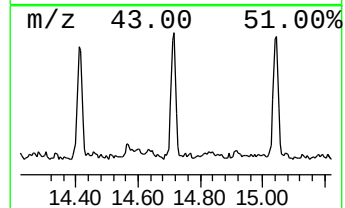
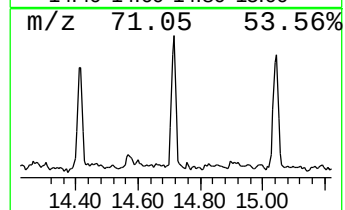
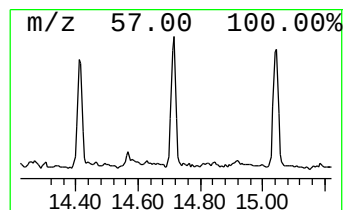
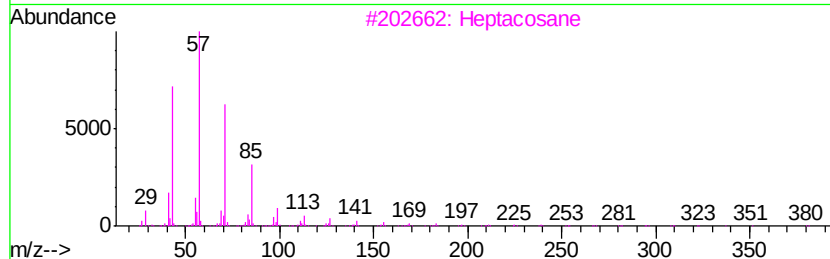
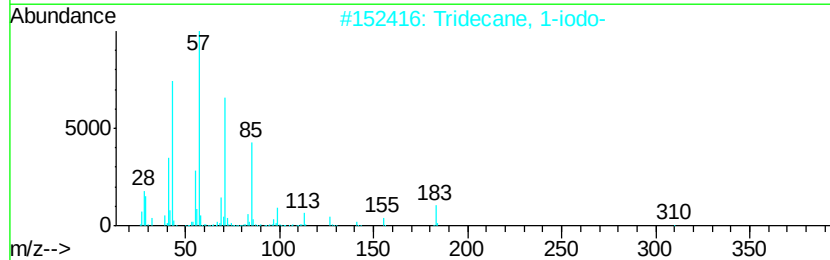
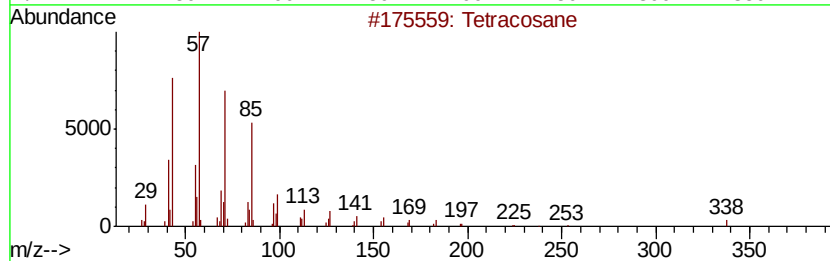
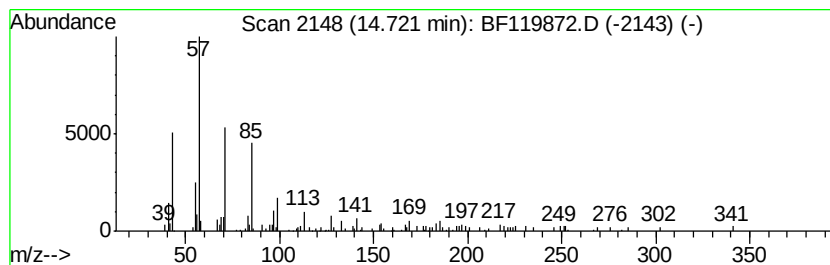
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	4.45 ng	177409	Perylene-d12	15.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	87
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
3			Heptacosane	380	C27H56	000593-49-7	83
4			Hexacosane	366	C26H54	000630-01-3	78
5			Hentriacontane	437	C31H64	000630-04-6	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040820\
Data File : BF119872.D
Acq On : 9 Apr 2020 16:30
Operator : MA/SJ
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Instrument :
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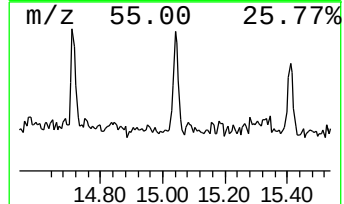
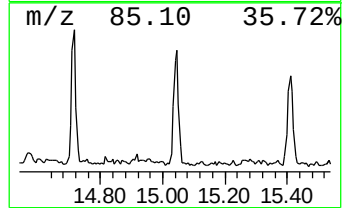
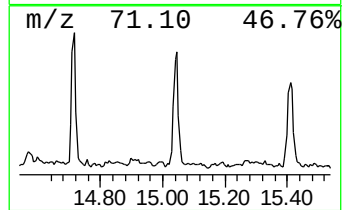
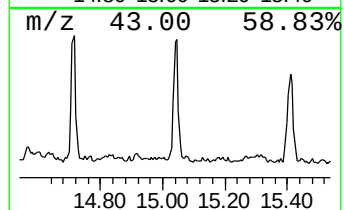
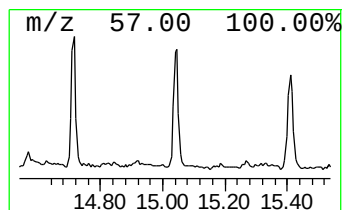
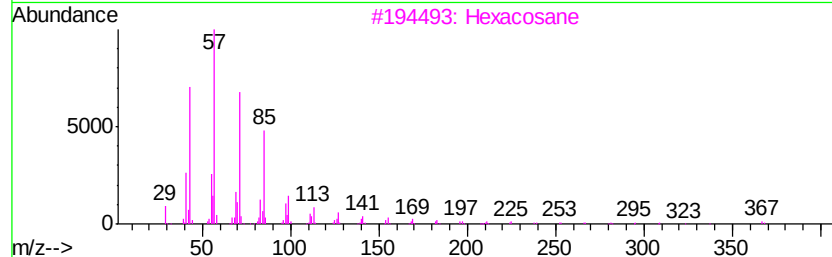
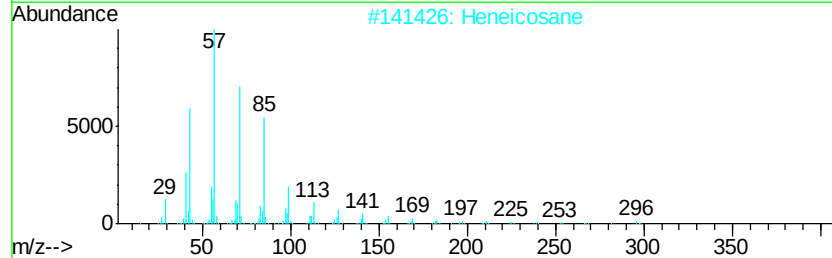
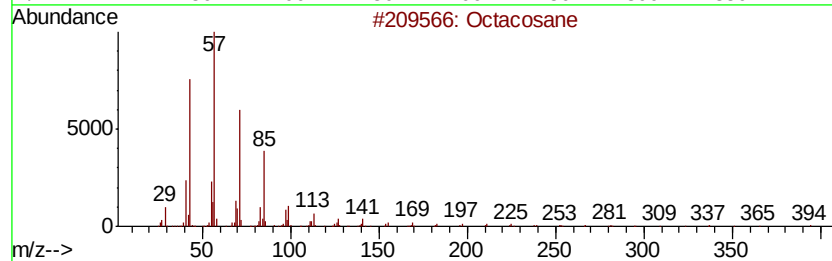
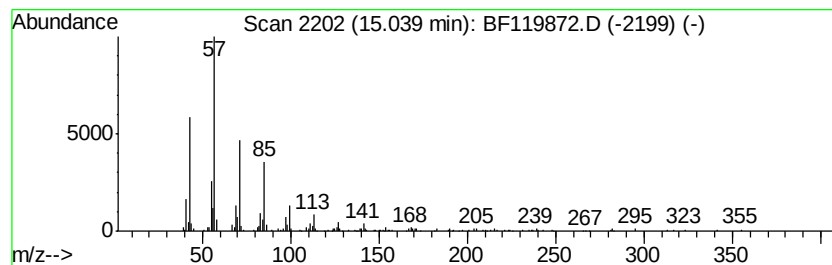
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	5.26 ng	209486	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Hexacosane	366	C26H54	000630-01-3	83
4		Eicosane	282	C20H42	000112-95-8	83
5		Octadecane	254	C18H38	000593-45-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040820\
Data File : BF119872.D
Acq On : 9 Apr 2020 16:30
Operator : MA/SJ
Sample : L2135-02
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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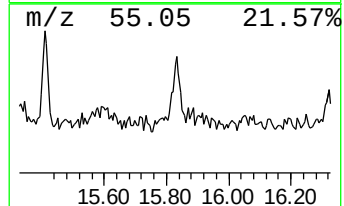
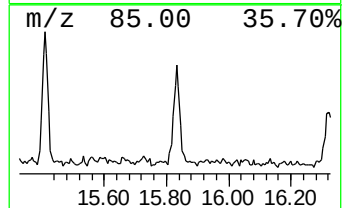
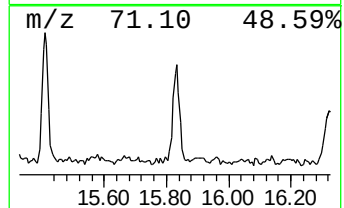
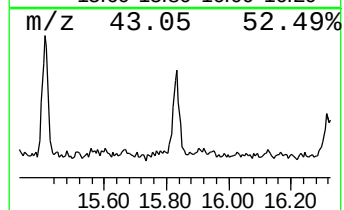
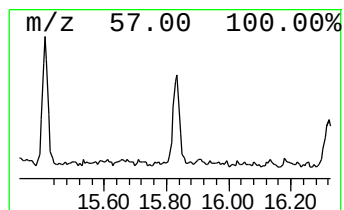
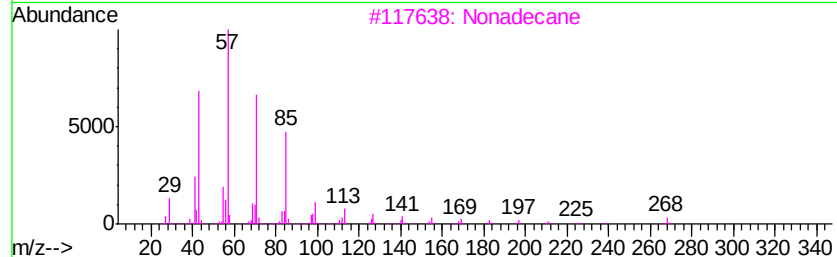
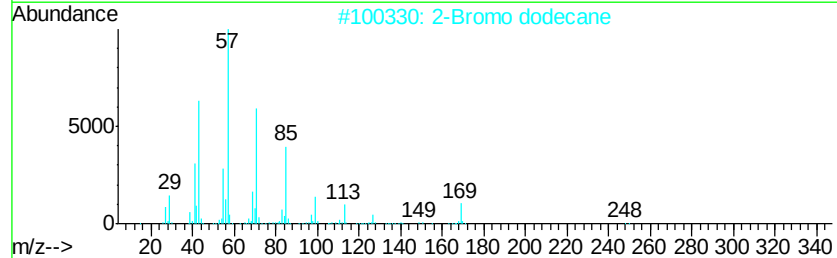
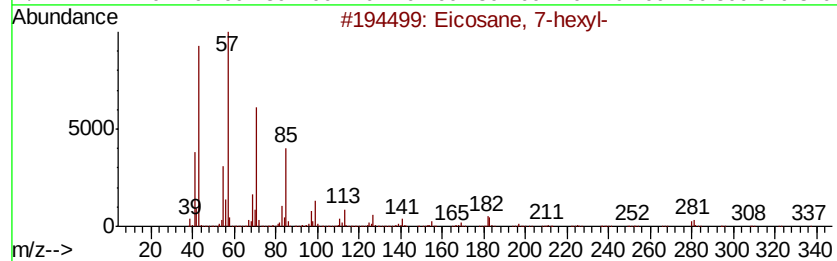
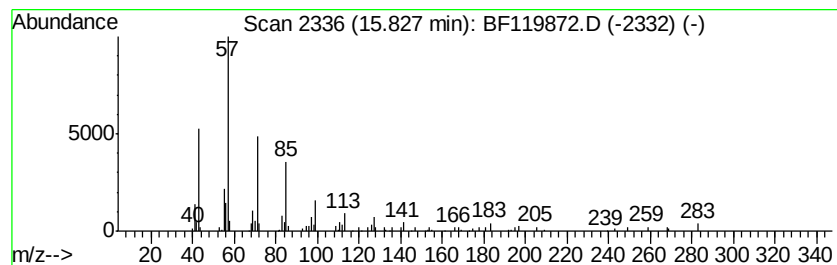
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Eicosane, 7-hexyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	3.64 ng	145199	Perylene-d12	15.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
2			2-Bromo dodecane	248	C12H25Br	013187-99-0	86
3			Nonadecane	268	C19H40	000629-92-5	86
4			Tetracosane	338	C24H50	000646-31-1	72
5			Heptadecane	240	C17H36	000629-78-7	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF040820\
Data File : BF119872.D
Acq On : 9 Apr 2020 16:30
Operator : MA/SJ
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ALS Vial : 39 Sample Multiplier: 1

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ClientSampleId :
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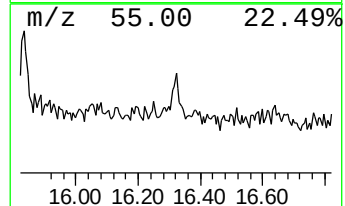
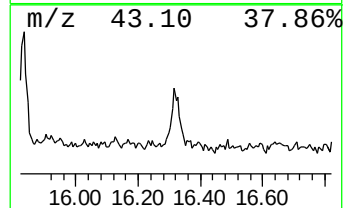
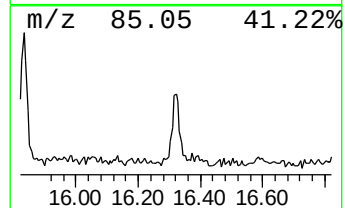
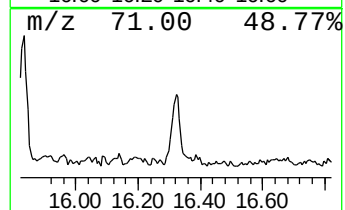
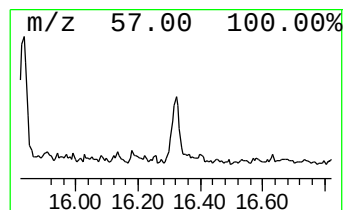
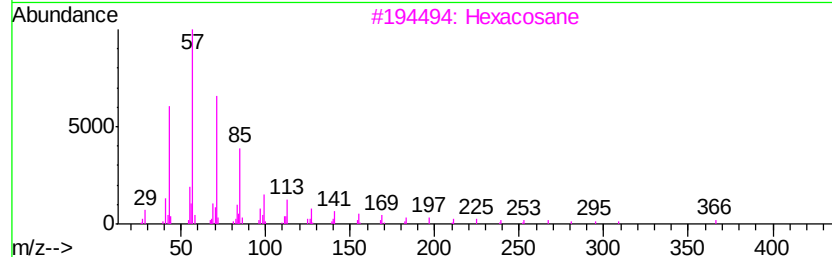
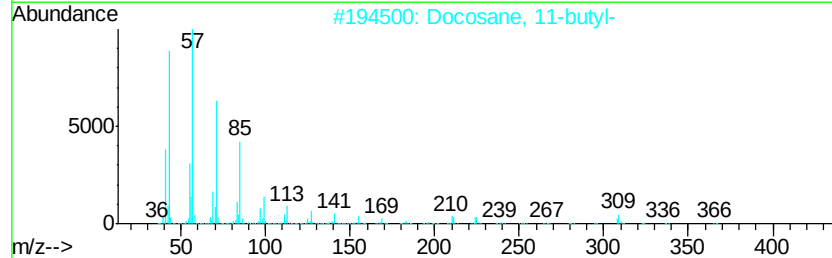
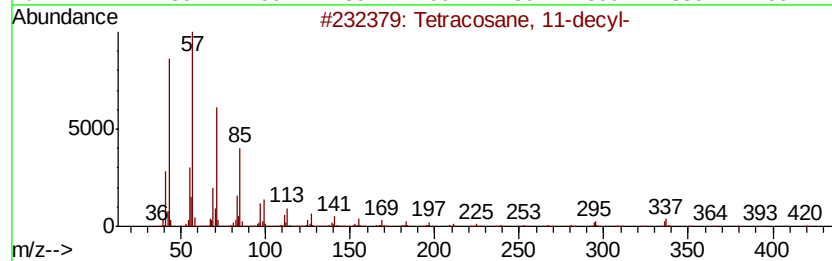
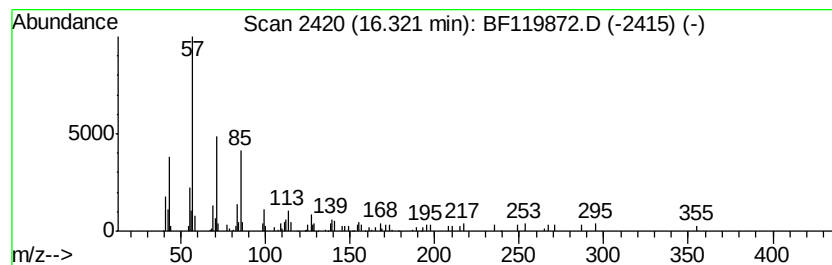
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Tetracosane, 11-decyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	2.20 ng	87676	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
2		Docosane, 11-butyl-	366	C26H54	013475-76-8	87
3		Hexacosane	366	C26H54	000630-01-3	87
4		Docosane, 11-decyl-	451	C32H66	055401-55-3	86
5		Heneicosane	296	C21H44	000629-94-7	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF040820\
 Data File : BF119872.D
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 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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n-Hexadecanoic acid	11.83	5.0	ng	334545	4	11.29	1331970	20.0
cis-Vaccenic acid	12.54	10.6	ng	702556	4	11.29	1331970	20.0
Octadecanoic acid	12.62	4.8	ng	212481	5	13.93	894259	20.0
unknown13.36	13.36	3.9	ng	175894	5	13.93	894259	20.0
Sulfurous acid, b...	13.79	4.9	ng	217854	5	13.93	894259	20.0
Heptadecane	14.11	2.4	ng	106628	5	13.93	894259	20.0
Eicosane	14.41	4.0	ng	179974	5	13.93	894259	20.0
Tetracosane	14.72	4.5	ng	177409	6	15.37	797236	20.0
Octacosane	15.04	5.3	ng	209486	6	15.37	797236	20.0
Eicosane, 7-hexyl-	15.83	3.6	ng	145199	6	15.37	797236	20.0
Tetracosane, 11-d...	16.32	2.2	ng	87676	6	15.37	797236	20.0